Experiments and Model Development for the Investigation of Sooting and Radiation Effects in Microgravity Droplet Combustion

Mun Young Choi and Ahmet Yozgatligil
Department of Mechanical Engineering and Mechanics
Drexel University, Philadelphia, PA 19104

Frederick L. Dryer and Andrei Kazakov
Mechanical and Aerospace Engineering
Princeton University, Princeton, NJ 08544

Ritsu Dobashi
Department of Chemical Systems Engineering
University of Tokyo
Tokyo, Japan

INTRODUCTION

Today, despite efforts to develop and utilize natural gas and renewable energy sources, nearly 97% of the energy used for transportation is derived from combustion of liquid fuels, principally derived from petroleum. While society continues to rely on liquid petroleum-based fuels as a major energy source in spite of their finite supply, it is of paramount importance to maximize the efficiency and minimize the environmental impact of the devices that burn these fuels. The development of improved energy conversion systems, having higher efficiencies and lower emissions, is central to meeting both local and regional air quality standards. This development requires improvements in computational design tools for applied energy conversion systems, which in turn requires more robust sub-model components for combustion chemistry, trasnport, energy transport (including radiation), and pollutant emissions (soot formation and burnout). The study of isolated droplet burning as a unidimensional, time dependent model diffusion flame system facilitates extensions of these mechanisms to include fuel molecular sizes and pollutants typical of conventional and alternative liquid fuels used in the transportation sector. Because of the simplified geometry, sub-model components from the most detailed to those reduced to sizes compatible for use in multi-dimensional, time dependent applied models can be developed, compared and validated against experimental diffusion flame processes, and tested against one another.

Based on observations in microgravity experiments on droplet combustion, it appears that the formation and lingering presence of soot within the fuel-rich region of isolated droplets can modify the burning rate [Choi et al., 1990; Jackson and Avedisian, 1994], flame structure and extinction [Nayagam et al., 1998; Marchese et al., 1999], soot aerosol properties [Manzello and Choi, 2001], and the effective thermophysical properties [Choi et al., 1990; Jackson and Avedisian, 1994]. These observations led to the belief that "perhaps one of the most important outstanding contributions of microgravity droplet combustion is the observation that in the absence of asymmetrical forced and natural convection, a soot shell is formed between the droplet surface and the flame, exerting an influence on the droplet combustion response far greater than previously recognized" [Law and Faeth, 1994]. The effects of soot on droplet burning parameters, including burning rate, soot shell dynamics, flame structure, and extinction phenomena provide significant testing parameters for studying the structure and coupling of soot models with other sub-model components.

OBJECTIVES OF STUDY

Microgravity droplet combustion is an ideal platform for advancing the understanding of diffusion flames of liquid hydrocarbon fuels and additives that are typically used in internal combustion engines and gas turbines. The burning of an isolated droplet is a robust problem that involves coupling of chemical reactions, multi-phase flow (liquid, gas, particulate) with phase change. The observations in previous microgravity investigations strongly suggest that a thorough interpretation of droplet burning behavior cannot be accomplished without examining and incorporating the influences of sooting and radiation. Experimental measurements will provide a robust test of the important interactions with burning rate, flame structure, flame extinction, and aerosol properties.

The development of detailed numerical modeling of spherically-symmetric droplet combustion provides opportunities to test and validate the chemical kinetic, transport, sooting, and radiation mechanisms for a realistic fuels under a variety of conditions that are unattainable by means other than those provided by microgravity. Improved mechanisms, especially the coupled gas-phase chemical kinetic and soot formation mechanisms for both n-heptane and ethanol fuels, are needed to integrate the influence of sooting in n-heptane combustion and to reconcile the recent discovery that ethanol flames produce significant soot under high pressures. Refinements of these models through comparison against well-characterized experiments performed in microgravity (for a wide range of residence times unattainable through any other geometrical configurations) can yield new and important understanding.

EXPERIMENT DESCRIPTION

The proposed experiments will consider two fuels: n-heptane, and ethanol. N-heptane is the simplest of liquid alkanes with properties similar to those found for conventional liquid fuels such as gasoline and distillates. Understanding of liquid ethanol combustion processes also has significant practical and fundamental implications. In recent years, the use of ethanol as a fuel additive has been stimulated by the Clean Air Act Amendments of 1990 [Vanderver, 1992] that require utilization of reformulated and oxygenated gasoline to reduce carbon monoxide and volatile organic compound emissions. With the phaseout of MTBE, ethanol remains one of the most favorable oxygenated additives. From the fundamental point of view, gas-phase oxidation chemistry for ethanol and n-heptane have been extensively studied. These factors make both valuable targets for fundamental droplet combustion studies and model validation that can ultimately lead to better understanding of practical liquid fuel combustion phenomena.

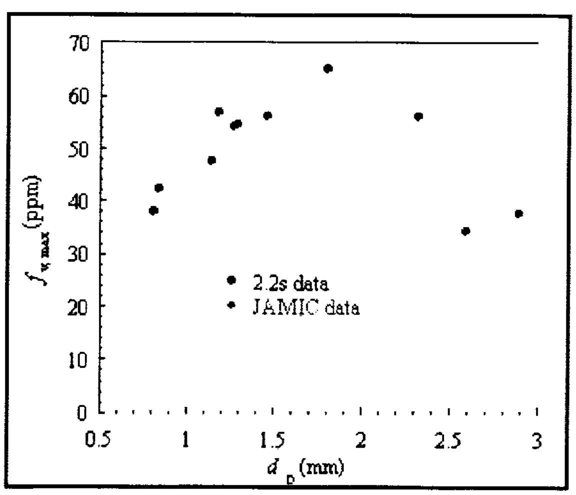
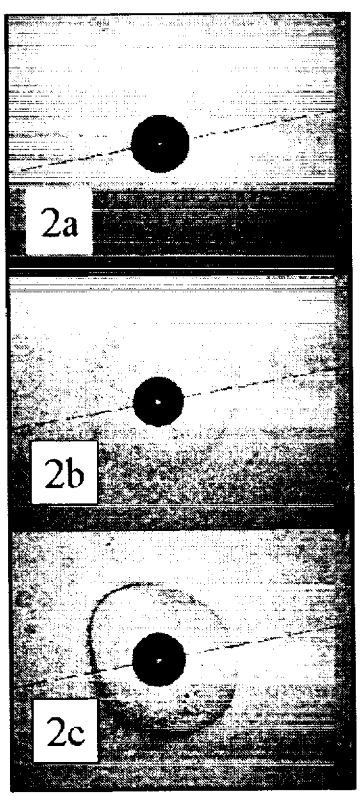


Figure 1

In these experiements, soot volume fraction will be measured using full-field light extinction at 635 nm. In this method, line of sight extinction measurements are deconvoluted using tomographic inversion [Dasch, 1992]. Soot temperature will be measured using line of sight flame emission data at two separate wavelengths (700 nm and 900 nm) with subsequent tomographic inversion. The ratio of the spectral emission intensity at each radial position will then be used for the application of two-wavelength pyrometry. This technique is similar to that used successfully in Laminar Soot Processes (LSP) Shuttle experiments. As in the LSP experiments, it is expected that due to the small soot particle sizes, the difference between the gas-temperature and the soot temperature will be small. Radiation from the flame will be measured using a broadband radiometer (detection spectrum ranging from 0.5 to 5 microns). Soot agglomerates will be sampled using a thermophoretic technique and analyzed using transmission electron microscopy. Ultraviolet emission due to hydroxyl radical chemiluminescence (and the interference from soot emission) occurring within the flame will be imaged using a Xybion intensified array CCD camera with a narrowband filter with central wavelength of 310 nm and a FWHM of 10 nm. This approach yields the instantaneous location of maximum OH^* emission which, in conjunction with detailed numerical modeling, will be used to define the transient flame structure.

RECENT PROGRESS

Soot volume fraction and radiative emission measurements for large droplet experiments were performed at the JAMIC 10 sec facility in Hokkaido, Japan. The maximum soot volume fraction, f_{vmax} values measured for the 2.6 mm and 2.9 mm initial droplet diameter experiments are plotted in **Figure 1** along with previous measurements for smaller droplets [Lee *et al.* 1998]. The maximum soot volume fractions for the larger droplets exhibit a significant departure from the linear increase as a function of d_0 as it might be inferred from the small droplet experiments. The measured maximum soot volume fractions for the larger droplets are nearly 40% smaller than the values obtained at d_0 = 1.8 mm. This reduction in sooting is expected to have strong implications on many aspects of the burning process. It is believed that increases in initial droplet diameter will produce radiative losses (due to both soot and non-luminous component) that will reduce the temperatures to below threshold temperatures required for additional soot formation. Results were presented and published in the *28th Symposium on Combustion* [Manzello et al., 2001].



Characterization of soot morphological properties including the primary particle size, d_p, radius of gyration, R_g, fractal dimension, D_f, and mass fractal prefactor term, k_f are important for the analysis of soot processes including particle growth, soot agglomeration and oxidation processes. Measurements of primary particle size and fractal dimensions for soot sampled in n-hexane droplet flames burning in microgravity flames are shown in Table I.

Table I			
	d_p (nm)	D_f	k_f
Normal-Gravity Soot	25.9	1.61	6.6
μg Soot at 0.5 sec	45.8	1.63	7.8

The increase in the primary particle dimensions with residence time is dramatic. The average primary particle size increased from 25.9 nm for soot collected in normal gravity to 45.8 nm for soot collected at 0.5s after ignition in microgravity. In the present experiments, the average k_f increased from 6.6 in normal gravity to 7.8 for the 0.5s microgravity experiment. D_f was nearly constant for normal-gravity and microgravity soot. Detailed results will appear in *the Int'l Journal of Heat and Mass Transfer* [Manzello and Choi, 2001].

As mentioned previously, ethanol has displayed unusual sooting characteristics that has not received much attention in the literature. As an oxygenate, ethanol is known to be essentially a non-sooting fuel at atmospheric pressures. At elevated pressures (starting from as low as 1.5 to 2 atm of air), however, an ethanol droplet flame has been shown to form soot [Yap, 1986]. High-pressure microgravity experiments using ethanol were performed at the JAMIC 10 sec. drop tower facilities. **Figure 2a** displays the back-lit view of an ethanol droplet burning in air at 1.8 atm. In **Figure 2b**, the pressure was increased to 2 atm and the oxygen concentration in nitrogen was increased to 0.25 mole fraction. The presence of the sootshell is clearly evident. In **Figure 2c**, the oxygen concentration was increased to 0.31 mole fraction while the pressure was maintained at 2 atm. The sootshell is more opaque (corresponding to higher soot concentration) and the luminosity of the flame was markedly brighter.

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